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ABSTRACT

We developed novel spectroscopic STM instruments for study of individual atom qubits.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

64. Relating atomic scale electronic phenomena to wave-like quasiparticle states in superconducting Bi2Sr2CaCu2O8+d K. McElroy, R. W. Simmonds, J. E. Hoffman, D.-H. Lee, J. Orenstein, H. Eisaki, S. Uchida & J.C. Davis., Nature 422, 520 (2003).
65. Incommensurate, dispersive, density of states modulations in Bi2Sr2CaCu2O8+ , K. McElroy, J. E. Hoffman, D. -H. Lee, K. M. Lang, H. Eisaki, S. Uchida and J. C. Davis." Physica C 388-389 , 225-226 (2003)
66. Vortex-induced quasi-particle `checkerboard' in Bi2Sr2CaCu2O8+ ", J. E. Hoffman, E. W. Hudson, K. M. Lang, H. Eisaki, S. Uchida and J. C. Davis. Physica C, 388-389,703 (2003).
67. Numerical Studies of the Superfluid Shapiro Effect". R. W. Simmonds, A. Marchenkov, J. C. Davis and R. E. Packard. Physica B 329, 63 (2003).
68. STM studies of individual Ti impurity atoms in Sr2RuO4", Barker BI, Dutta SK, Lupien C, McEuen PL, Kikugawa N, Maeno Y, Davis JC PHYSICA B 329: 1334 (2003)
69. Fourier Transform Scanning Tunneling Spectroscopy Studies of the Electronic Structure of Superconducting Bi2Sr2CaCu2O8+d", K. McElroy, J. E. Hoffman H. Eisaki S. Uchida & J.C. Davis, AIP CONFERENCE PROCEEDINGS 696, 1 (2003).
70. Fourier-transform scanning tunneling spectroscopy: A new window on the electronic structure of Bi2Sr2CaCu2O8+d" Davis JC. ACTA. PHYS. POL. A 104 (3-4): 193-204 (2003).
71. Measurements of attenuation of third sound: Evidence of trapped vorticity in thick films of superfluid He-4 Hoffman, J A, Penanen K, Davis J.C. et al J LOW TEMP PHYS 135: 177-202 (2004).
72. "Effect of 3He on Third Sound Attenuation in Thick 4He Films"
Hoffman, J A, Penanen K, Davis J.C. et al J LOW TEMP PHYS 134: 1069 (2004).
73. A 'checkerboard' electronic crystal state in Lightly Hole-Doped Ca2-xNaxCuO2Cl¬2" T. Hanaguri, C. Lupien, Y. Kohsaka, D.-H. Lee, M. Azuma, M. Takano, H. Takagi, & J. C. Davis. Nature 430, 1001 (2004).
74. Coincidence of 'checkerboard' charge order and antinodal state
decoherence in strongly underdoped superconducting Bi2Sr2CaCu2O8+?, K. McElroy, D.-H. Lee, J.E. Hoffman, K.M. Lang, J. Lee, H Esiaki, S Uchida, & J.C. Davis, Phys. Rev. Lett. 94, 197005 (2005).
75. 'Wavefunction Imaging' Studies of High-Tc Superconductivity, J. Slezak, J. Lee and J. C. Davis, MRS Bulletin 30, 437 (2005).
76. 'Spectroscopic Imaging STM Studies of High-Tc Superconductivity' Jinho Lee et al , J. Phys. Chem. Solids 66 , 1370 (2005).
77. Atomic-scale Sources and Mechanism of Nanoscale Electronic Disorder in Bi2212. K. McElroy, Jinho Lee, James Slezak, D.-H. Lee, H. Eisaki, S. Uchida, J.C. Davis. Science 309, 1048 (2005).

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Number of Inventions:

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Millikelvin STM for exploration of Single Atom Qubit Physics

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Scanning tunneling microscopy (STM) is most famous for its ability to provide an image of the location of ach atom on a surface. This ‘topographic’ capability exists because the rate of electron tunneling through vacuum depends exponentially on the tip/sample distance with an exponential decay length of 1 Å for typical situations. Therefore, when the tunneling current is held constant while the STM tip moves laterally across the surface, the elevation of the tip at each location provides a topographic ‘image’ of the surface. However, STM has a much more important and profound capability beyond topographic imaging. This is its ability to measure the local density of electronic states (LDOS) with atomic precision. This capability is described in Fig. 1 below.

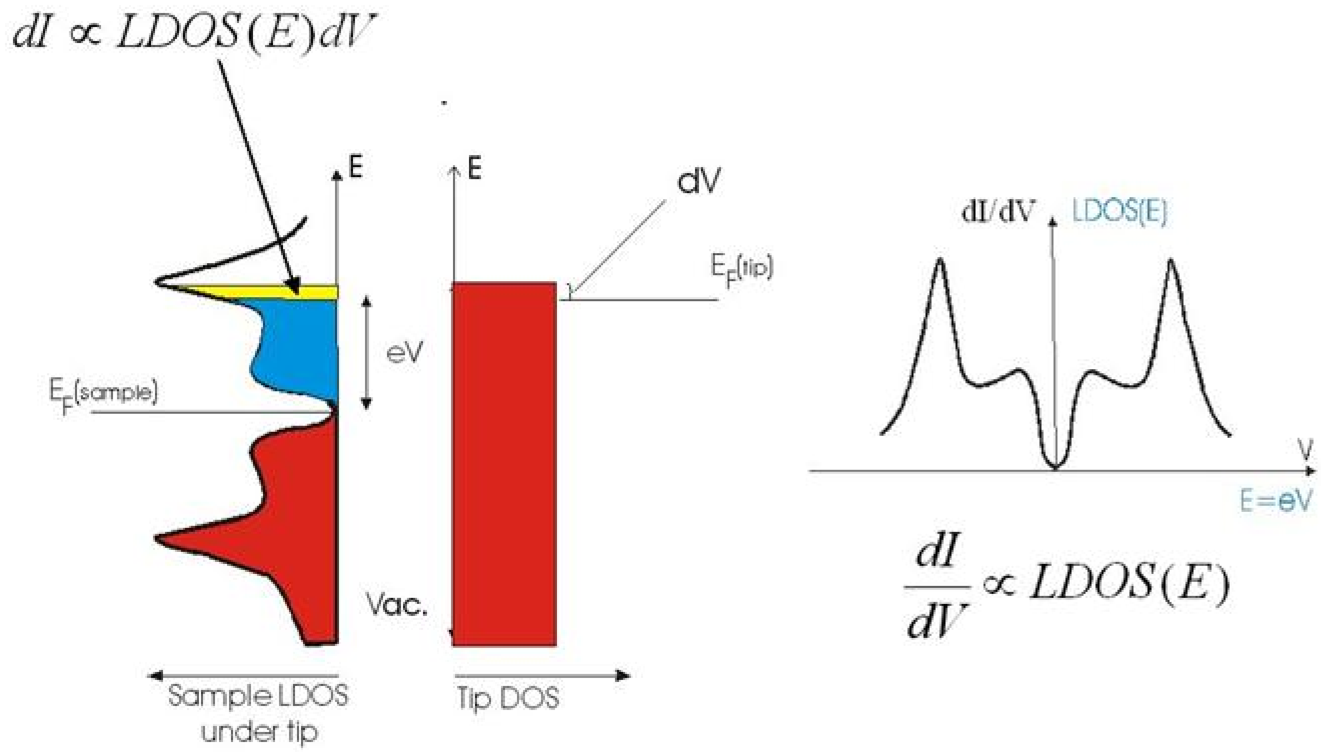

Figure 1. *A schematic diagram of the LDOS (horizontal axis) as a function of energy (vertical axis) in a sample material in tunneling contact with the STM tip. The tip LDOS is assumed independent of energy.)The Fermi level of the tip is raised by increasing the positive bias voltage on the sample relative to it. The blue states in the sample are those into which the electrons tunnel. When the tip bias is incremented by dV, the tunneling current increments by dI which is proportional to the sample LDOS at the energy eV. Thus a plot of dI/dV versus V yields a plot of LDOS (E).*

At a fixed location of the tip, the differential tunneling conductance dI/dV measures the additional tunneling current occurring between the voltage V (between the sample and tip) and V+dV. In Fig. 4 we show schematically how this happens. When the tip Fermi-level is lifted by an amount dE=edV upon changing the sample bias by dV, new empty states in the sample (shown in yellow) become available for tunneling. The density of these states is the LDOS at energy eV above the Fermi-level of the sample. Therefore, by measuring dI/dV as a function of V at very low temperatures, one can measure the LDOS as a function of E in the sample.

We have recently developed new techniques for measuring dI/dV as a function both of E and of location in the sample with sub-atomic resolution[1]. This is in fact an extremely difficult thing to do, since it relies on stabilizing the tip at a predetermined series of locations relative to the surface, controlled with picometer precision, without using feedback. This capability is vital to since it allows one to map the electronic structure of even the most inhomogeneous sample with atomic precision.

The qubit at a single dopant atom in a semiconductor is based on the two Zeeman split (and thus opposite spin) states at the dopant atom in high magnetic field at low temperatures. Spin-split electronic states at individual *magnetic* impurity atoms have long been predicted in high-T_c systems[2] even in the absence of an external field. This situation is shown schematically in Figure 2a and 2b. There is no external magnetic field here but the spin-splitting occurs because there is a very large *local* field due to the moment at the Ni atom. If the magnetic interaction energy W (the exchange energy between the impurity moment and the electrons) were zero, the expected LDOS spectrum at this site would be a peak at positive energy Ω. However, a non-zero magnetic interaction energy W of the electrons with the moment of the magnetic impurity atom, should split the state into two spin-polarized states at energies Ω_1 (spin-down) and Ω_2 (spin-up) as shown schematically in Fig. 2b. The existence of distinct spin-up and spin-down bound-states at a single magnetic dopant atom in a high-Tc material would therefore become apparent as *two* peaks in dI/dV as shown in Fig. 2b.

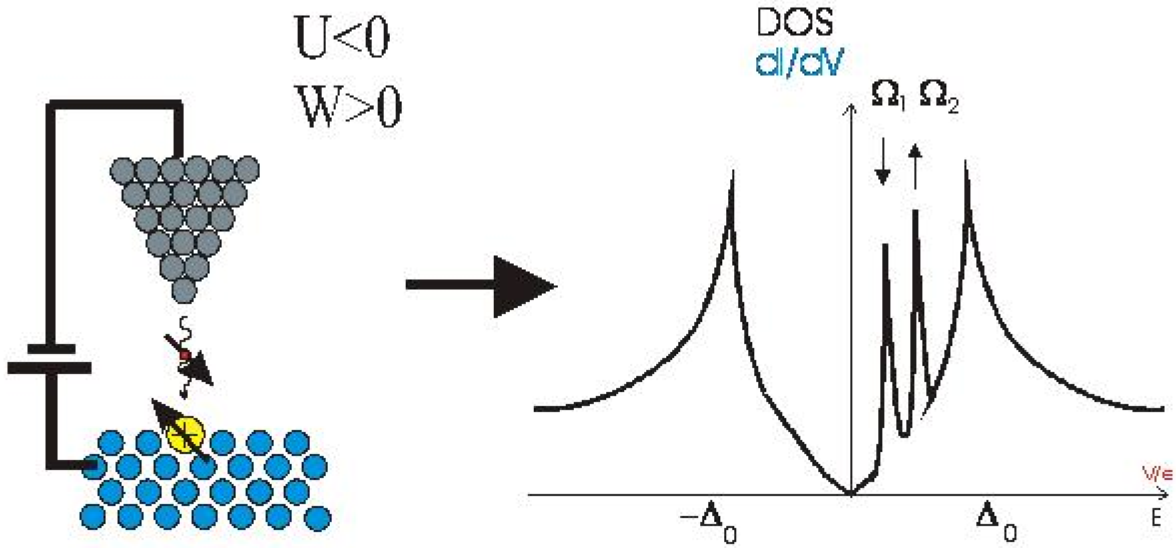

Figure 2a. *A schematic diagram of the STM tip parked above the magnetic dopant atom in a high-Tc superconductor.* ***b*** *The theoretically predicted tunneling spectrum showing the V-shaped gap in the LDOS of a pure high-Tc superconductor plus two intra-gap states* $\left|\uparrow\right\rangle$ *and* $\left|\downarrow\right\rangle$**.**

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Experimentally, this is precisely what we have recently discovered[3]. Figure 3 shows the spectrum measured at the Ni impurity atom site in red. It is dominated by of two peaks at positive bias (Ω_1=9meV and Ω_2=19meV). One is the $\left|\uparrow\right\rangle$ level and the other is $\left|\downarrow\right\rangle$.

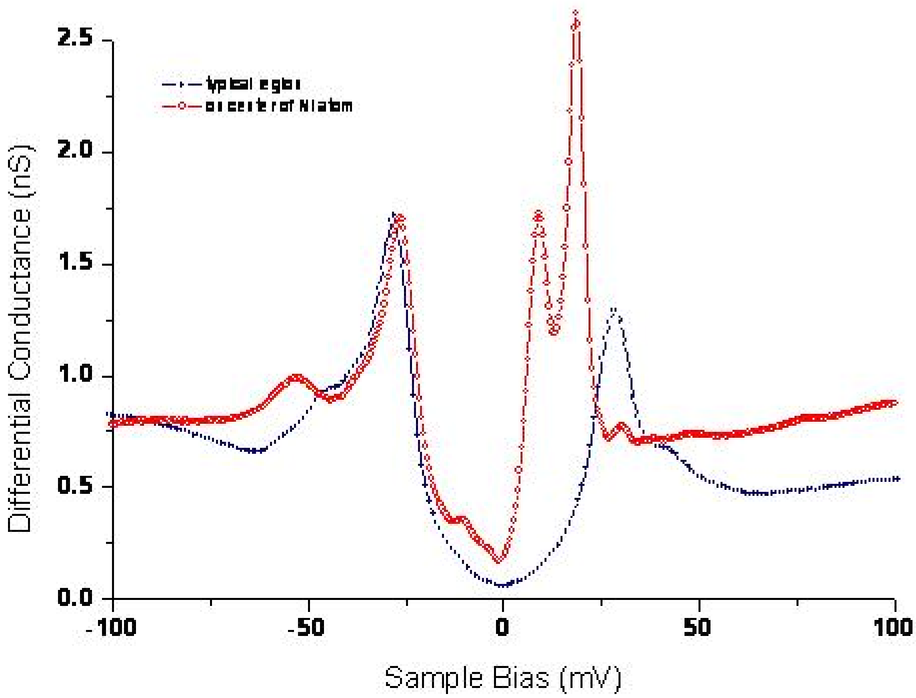

Figure 3. The red line is the measured LDOS spectrum at the Ni atom site in BSCCO showing the two spin split local states. The blue curve is the unperturbed high-Tc LDOS spectrum.

These results are significant for several reasons. First they demonstrate that it is physically possible to measure the energy level spectrum of electronic states at *individual* impurity atoms by using low temperature scanning tunneling spectroscopy. Therefore, tunneling spectroscopy can now be applied to measurement of dopant atom bound-state properties for quantum computing studies. Second, the $|\uparrow\rangle$ and $|\downarrow\rangle$ levels of a bound-state at a *single* dopant atom have been observed for the first time. Electronic measurement of the spin of a single-atom bound-state can therefore be contemplated in the context of quantum computing.

In principle one could, by using these newly developed STM techniques, directly test whether many of the electronic manipulations of states at individual dopant atoms proposed by Kane or DiVincenzo can be made at single dopant atoms in Si (or other semiconductor). To do so, an STM operating in spectroscopic mode, at very high magnetic fields, at temperatures near

100mK, with picometer spatial resolution, while retaining an identifiable single atom in the field of view, is required. These are extremely demanding specifications - far beyond that of any commercial STM system. However, all of the required STM technology has recently been developed by the Davis Group through the support of the ARO4. We proposed to use these unique STM capabilities to carry out studies of electronic bound-states at individual ^{31}P (and other) atoms in Si (and other semiconductors).

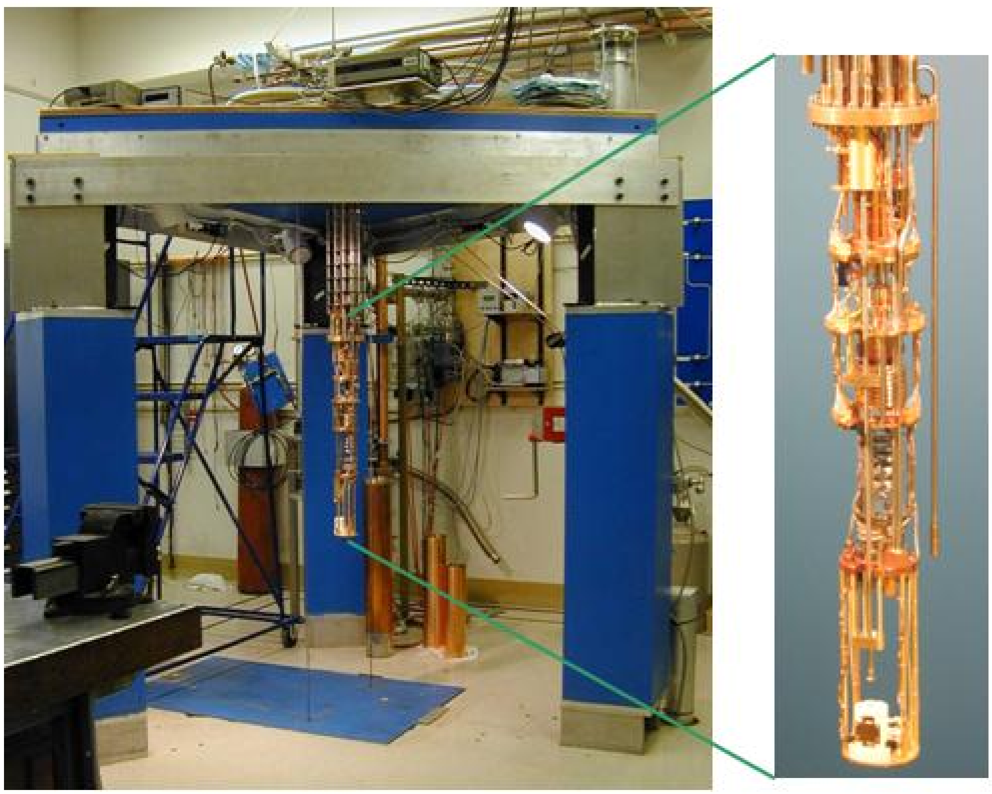

Fig.4. Picture of the vibration isolation cryostat including the dilution refrigerator with STM head suspended below the mixing chamber.

The first achievement was successful development of a system (Fig. 4) that allows atomic resolution spectroscopic mapping STM at temperatures down to 12mK in fields up to 9 Tesla. This is the only system of this type in the world.

We are now applying this millikelvin, high-field, scanning tunneling microcopy (STM) to study the fundamental physics of bound electronic states at individual dopant atoms in a semiconductor. Although much has been said and written about electronically addressing single quantum states at dopant atoms in semiconductors, no experiments have been carried out and little is known about the applied physics of this situation. Therefore our studies are initially directed towards direct detection and study of the bound-states at individual dopant Te atoms (in high magnetic fields at very low temperatures) in GaAs as a test case.

Our initial studies show that we can identify each Te atom location (Fig. 5), measure their spectrum (Fig. 6), and locally map the wavefunction of the donor state with spectroscopic mapping (Fig. 6).

Fig. 5. Images of <110> surface of GaAs showing surface electronic defect states and the location of the Te donor atoms.

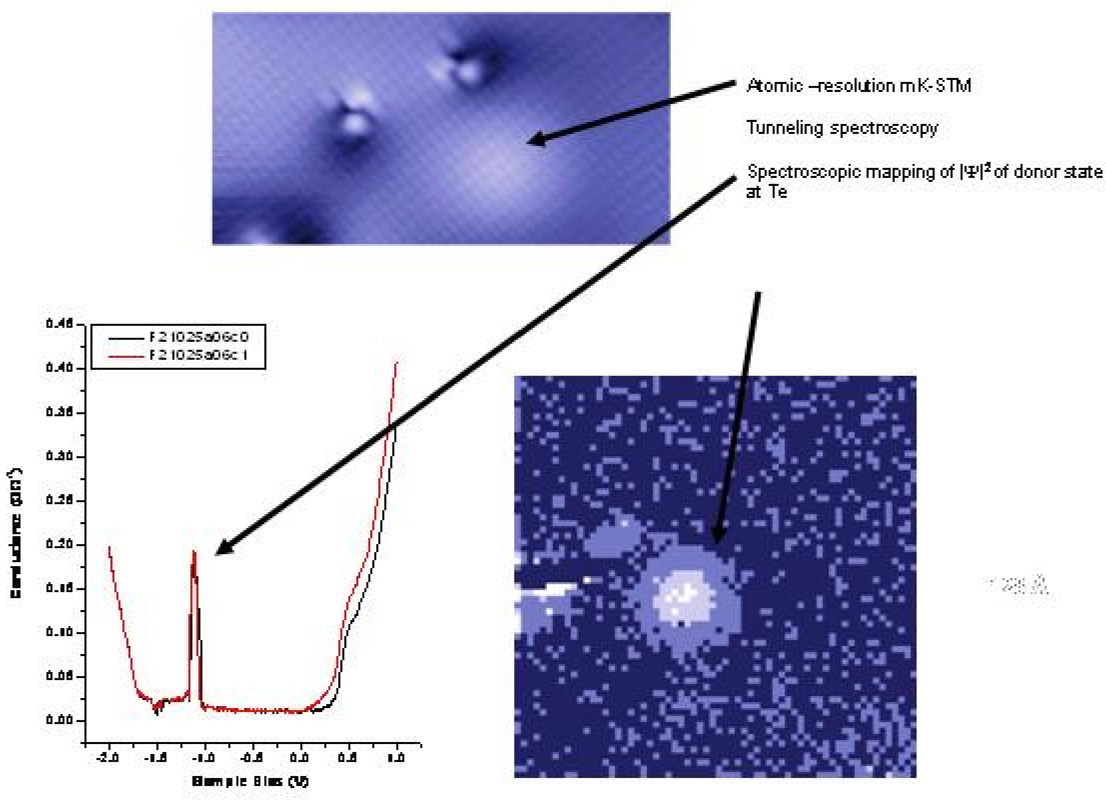

Fig. 6. Combination topographic image, spectrum at the Te site, and wavefunction image of the Te donor state (taken at 25 mK).

There is another very promising opportunity for detection of local spin polarized states at an individual dopant atom. In a conventional s-wave superconductor a local state exists at every magnetic impurity atoms. This state is split by local magnetic interactions like those described in Fig. 2 but now in a fully gapped superconducting system. Again the temperature necessary to resolve these states is well below 1K for conventional low temperature superconductors. We use $NbSe_2$ as the substrate because it is a low temperature superconducting system with almost perfect atomic surfaces.

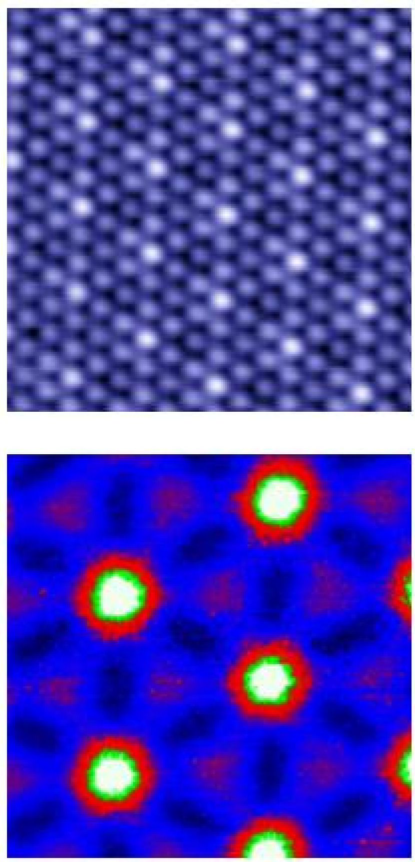

Fig. 7. a 250 Å square topographic image of the Se surface of $NbSe_2$. Each Se atom, plus the charge density wave modulations, are seen. b. Wavefunction image of the vortex core states in a 1200 Å FOV at B~2 tesla.

We intercalate magnetic impurity atoms (Fe) between the planes and then, when we cleave it in cryogenic vacuum, they remain on the top surface. We can manipulate these atoms to make magnetic nanostructures whose electronic wavefunctions we are now studying by spectroscopic mapping at mK temperatures. Spectroscopic studies do indeed reveal local states at these atoms which are consistent with theory. Further studies are planned to pursue this exciting opportunity with different magnetic atoms (Co, Mn and Fe) in this system.

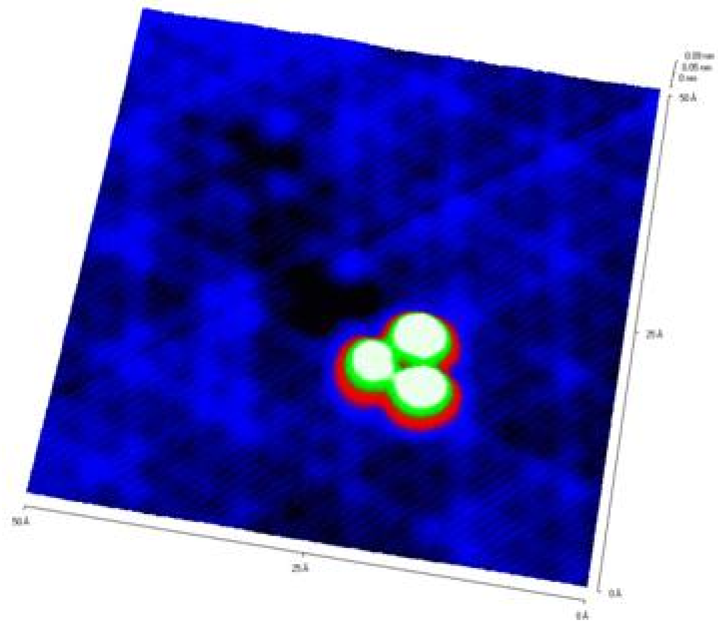

Fig. 8. A magnetic cluster of 3 Fe atoms assembled on the $NbSe_2$ surface.

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